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Electron capture in $H^+ - O$ collisions

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Abstract . Cross sections for one electron capture in proton-oxygen collisions are calculated by applying two center atomic state expansion method in the energy range of 0.1 to 300 keV. Slater type orbitals are used to represent the ground state wave function of oxygen atom, obtained from the model potential. Comparisons have been made with the existing theoretical findings as well as with the experimental data. The present calculated values are found to be encouraging.

Keywords Electron capture, model potential, Slater type orbital

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1. Introduction

Charge transfer process including heavy particles is one of the main subjects of recent theoretical and experimental investigations on ion-atom collisions due to its practical applications in many areas of physics. Theoretical studies of this process are mostly concerned with the mono-electron target such as hydrogen. However, few calculations are available for the systems involving multi-electron targets, for example, the collision of proton with atomic oxygen; this system is the subject of the present study.

This particular type of reaction has a great importance for energy loss processes in the outer atmosphere of Earth. At heights above few hundred kilometers, atomic oxygen has a much higher density in comparison with N_2 and O_2 and the cross sections involving proton–oxygen thus have a particular geophysical importance [1]. In addition, a detailed understanding of the complex way in which energetic ions of extra-terrestrial origin interact with earth atmosphere continues to be of considerable interest.

As oxygen has in the outermost shell, four electrons in $2p$ subshell and two electrons in $2s$ subshell, the theoretical treatment of all the outer shell electrons as such, is a formidable task. From the theoretical stand point, the loosely bound valence electron may be considered to move in an effective central potential established by O^+ ($1s^2 2s^2 2p^3$) core. The problem then can be simplified as one electron problem. In early years, such treatment of multi-electron targets have been reported by many theoreticians [2]

In 1964, Stebbings *et al* [3] have used a modulated crossed beam technique employing an RF dicharge source of partially dissociated oxygen to measure the charge transfer cross sections of proton-oxygen system in the energy range of 0.04 to 10 keV. Rutherford and Vroom [4] in 1974, measured the charge transfer cross sections of the above system using a modulated crossed beam technique in the energy range of 1 to 500 eV. In this technique, oxygen beam was derived from the iridium tube furnace. Williams *et al* [5] in a different experimental approach, used iridium furnace to provide a partially dissociated oxygen. They considered the energy range of 2.5 to 25 keV and obtained 50% of the values measured by Stebbings *et al* [3]. However, in a more recent crossed beam experiment, Van Zyl and Steven [6] measured capture cross sections, which are found to be in good agreement with the data of Ref. [3].

Absolute differential cross sections have been measured by Lindsay *et al* [7] for proton collision with atomic oxygen.

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These measurements were made using a flowing gas target, which consisted of a mixture of atomic and molecular oxygen produced by passage of O_2 through a microwave discharge. They obtained the cross sections by subtracting the signal due to molecular oxygen from that due to the mixture of O and O_2. Their measurements are found to be in reasonable accord with Ref. [3]. Thompson *et al* [8] used a crossed beam technique incorporating time of flight analysis and coincidence counting of the collision products to study one-electron capture by 6–100 keV proton in collision with oxygen atom derived from iridium tube furnace. This recent experiment has provided impetus for the theoreticians to calculate the cross sections at least in good agreement with experimental data.

Kimura *et al* [9] calculated theoretically, the cross sections of proton-oxygen collision in the energy range of 10 to 10^3 eV using the molecular orbital expansion method. The molecular state expansion method is best suited in the very low-energy region. We know that when the relative velocity of the colliding particles is considerably low, nearly of the order of orbital velocity of the bound electron, the molecular expansion method produces reliable results. For increased projectile energies, the molecular state expansion method is no longer valid and then the two-center atomic state expansion method is suitable to study the electron capture processes in ion-atom collisions. More recently, Hamre *et al* [1] have calculated the one-electron capture, excitation and ionization in proton-oxygen collisions. They have represented the electronic states of oxygen atom by orbitals obtained from the analytical model potential and have reported that capture cross sections are dominated by $2p$ electrons.

In the present article, we have applied the two-center atomic state expansion method to study proton-oxygen collision.

2. Theory

We adopt the impact parameter formalism where the projectile (A) and the target (B) move in equal and opposite velocities $v/2$, v being the relative velocity. The mid-point of the line joining the two nuclei is chosen as origin. Let $\boldsymbol{R}$ ($= \boldsymbol{p} + vt$, $\boldsymbol{p}$ is the impact parameter), be the position vector of the projectile relative to the target and $\boldsymbol{r}_p$, $\boldsymbol{r}_t$ and $\boldsymbol{r}$ be the position vectors of the electron relative to the projectile, target, and the origin, respectively.

We know, when the relative velocity between the nuclei is not small compared to the orbital velocity of the electron, the molecular state expansion method is not appropriate to study the electron capture processes. In that case, it is useful to consider the total wave function for the system ($A^+B^+e^-$) in terms of the eigen-functions of the atoms (A^+e^-) and (B^+e^-). Although the eigen function of any one of the two atoms form a complete set, the necessity of truncation makes it advantageous to use expansion in terms of the eigen functions of both the atoms. The problem is thus simplified to that of finding the solution of the time dependent Schrödinger equation for the electron with appropriate initial condition. Thus, the two-center atomic state expansion method produces correct results for charge transfer at intermediate and high energies. The method adopted here is described below briefly.

Initially, the electron is bound to oxygen atom in its ground state. Time is measured from the instant when two nuclei are closest to each other. Initially at $t = -\infty$, Ψ must represent a condition in which the electron is attached to oxygen in its ground state. The probability of electron capture by proton in the final state is to be obtained by solving

$$H\Psi = i\,\partial\Psi/\partial t \tag{1}$$

and finding Ψ at $t = +\infty$.

The eq. (1) may be obtained by making the following integral

$$I = \frac{1}{2}\int\left[\Psi^* H\Psi + \Psi H\Psi^* - i\Psi^*\frac{\partial\Psi}{\partial t} - i\Psi\frac{\partial\Psi^*}{\partial t}\right]dv\,dt \tag{2}$$

stationary with respect to small arbitrary variation of Ψ and its complex conjugate Ψ^*.

(atomic units are considered throughout)

We now approximate Ψ as a trial wave function

$$\Psi_t = a_1(t)\Psi_1 + a_2(t)\Psi_2,$$

where Ψ_1 and Ψ_2 are the ground state wave functions around oxygen and hydrogen atom respectively. Now, the wave function around the oxygen atom can be written in the form of

$$\psi_1 = \phi_1(r_t)\exp\left(it + \frac{i}{8}v^2 t\right), \tag{3}$$

where $\phi_1(r_t) = \sum c_l^{n_l} e^{-\beta_l r_t}\, r_t^{l}\, Y_{lm}(r_t)$,

c_l and β_l are the coefficients and the exponent of the Slater orbitals. The model potential used in the present work is of the form

$$V = -\frac{1}{r_t} - \frac{\exp(-2.067\, r_t)}{r_t}\{7 + 1.323\, r_t\}. \tag{4}$$

This model potential contains two parts, first part represents the long-range Coulomb potential and the second part represents short range potential. When we treat the multi-electron target atom as one electron atom, the other electrons make a core with the nuclei where the effects of distortion, correlation *etc* are present. These are represented by the short range part of the model potential and the effective (excited) electron effect is represented by the long range part of this potential. So the bound state wave functions of multi-electron target atoms are represented by Slater type orbitals obtained from this model potential and have reported

encouraging results. It may be pointed out that the model potential used in Ref. [1] is of different type. We have retained the second order correction term in the potential. However, both the model potentials satisfy the correct boundary conditions. In the present case, the arbitrary parameters are chosen variationally with respect to Slater basis set in such a way that the corresponding Hamiltonian of the active electron is diagonalized to reproduce correct binding energy. The binding energy of the active electron on target ion is calculated from the tables of Clementi and Roetti [10]. To check the accuracy of the wave function, virial theorem has been tested, and is found to be accurate within 0.01%. This type of model potential has been used by various authors [11–13]

Further substituting Ψ'_f for Ψ' is eq. (2) and minimizing the variation integral for small arbitrary variation of a_1^* and a_2^*, we get the coupled differential equations and are solved numerically by Runge-Kutta method. It is seen that the unitarity of $\int \Psi_f^* \Psi_f \, dr'$ is preserved at all times and we employ this fact as a check on the solutions of differential equations, at any instant. Finally, the squares of the absolute values the coefficients a_1 and a_2 at time t give the probabilities

Now the total capture cross section (Q_c) may be computed by performing the following integral

$$Q_c = 2\pi \int |a_2(t \qquad p dp$$

3. Results and discussion

The results for capture cross sections calculated by the present approach are presented in Figure 1. For comparison,

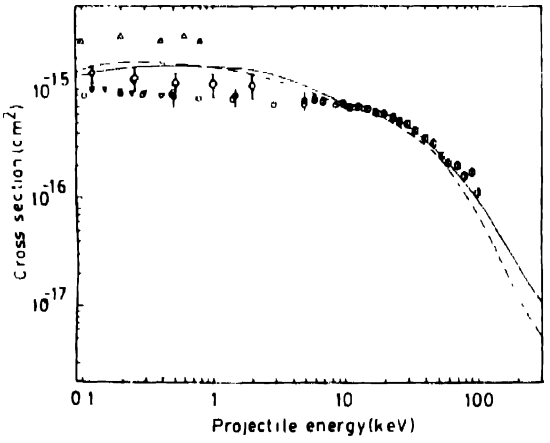

Figure 1. Total cross sections for electron capture in p-O collisions. Present result (- - -). Hamre *et al* [1] (— — —) Kimura *et al* [9] (Δ Δ) Expt. data Van Zyl and Steven [6] (◊ ◊). Thompson *et al* [8] (□□). Stebbings *et al* [3] (○ ○). Lindsay *et al* [7] (●●) Rutherford and Vroom [4] (▽ ▽)

we have also presented other existing theoretical values as well as the experimental data in the same figure. On comparison, it is evident from the figure that the present values overestimate the experimental data of Stebbings *et al* [3], Lindsay *et al* [7] and Rutherford and Vroom [4] in the low impact energy region, particularly at 0.1 to 8 keV. However, the present values are found to be closer to the data obtained in Ref. [6]. Also, the present results are found to interpret well the experimental data of Thompson *et al* [8] in the energy range 10–100 keV. However, below this energy range, the present results are found to be higher in magnitude

The calculated values of Kimura *et al* [9] are found to be higher in magnitude in comparison with the present theoretical values as well as the experiment data presented in the figure. The more recent values of Hamre *et al* [1] are found to be slightly smaller in magnitude in comparison with the present calculated values in the energy range of 0.6 to 300 keV. Below 0.6 keV, the present results although smaller in magnitude in comparison with the results of Hamre *et al* [1], agree reasonably well with the experimental data of Van Zyl *et al* [6]. In the range of 0.1 to 2 keV, the overall agreement of the present results and those of Ref. [1] with the experiment are almost equally good.

It is interesting to note that the present results for capture cross sections are found to reproduce reasonably well the more recent experimental data of Thompson *et al* [8] at higher energies in comparison with the values of Hamre *et al* [1] who used the atomic state expansion method like ours but with a different model potential. It is well known from the work of Madison [14] that the theoretical models for the collision problems are sensitive to the quality of the target wave function. As such, it is of current interest to describe the target wave function more accurately.

4. Conclusion

We have computed the total cross sections for the charge transfer reaction of proton-oxygen collisions. Applying the one electron approximation to this particular type of collision process, we have obtained results which are in reasonably good agreement with the experimental data in the intermediate energy region. The present calculation with the Coulomb-Yukawa potential of the type of eq. (4) thus makes a significant contribution for predicting reasonably accurate values of the cross sections in the intermediate impact energy region. However, it is observed from Figure 1 that none of the theories agree well with the experiments in the low energy region concerned, and a more detailed study of the system, particularly in the low energy region, is required.

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